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A coarse-grained computational model of DNA from all-atom molecular dynamics simulations. GAREGIN PAPOIAN, ALEXEY SAVELYEV, The University of North Carolina at Chapel Hill — DNA folds into a highly compact chromatin structure in the eukariotic cells. Counterions and the aqueous solvent provide a stabilizing medium for the maintanence of the highly compact and organized DNA structures. Thus, detailed understanding of counterion condensation around DNA is required to build a coarse-grained computational model of a chromatin fiber. We carried out large-scale all-atom Molecular Dynamics simulations of a 16-mer DNA in explicit water with Na+ and K+ counterions to gain insight into generic aspects of monovalent counterion condensation around the whole DNA molecule, focusing on the discrete nature of water and ions. We found that the Na+ ions penetrate the DNA interior and condense around the DNA exterior to a significantly larger degree compared with the K+ ions. We have provided a microscopic explanation for the larger Na+ affinity towards DNA, that is based on a combination of steric, electrostatic, and hydration effects. Our simulations are consistent with the prior DNA compaction and electrophoretic mobility experiments. We developed a coarse-grained DNA model based on the results of these all-atom simulations.

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